TAKAGI FACTORIZATION OF MATRICES DEPENDING ON PARAMETERS AND LOCATING DEGENERACIES OF SINGULAR VALUES

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ABSTRACT. In this work we consider the Takagi factorization of a matrix valued function depending on parameters. We give smoothness and genericity results and pay particular attention to the concerns caused by having either a singular value equal to 0 or multiple singular values. For these phenomena, we give theoretical results showing that their co-dimension is 2, and we further develop and test numerical methods to locate in parameter space values where these occurrences take place. Numerical study of the density of these occurrences is performed.

1. INTRODUCTION. TAKAGI FACTORIZATION OF A MATRIX.

The Takagi factorization is concerned with complex symmetric matrices, that is one has $A \in \mathbb{C}^{n \times n}$, $A^T = A$, and seeks the factorization $A = USU^T$, where $U \in \mathbb{C}^{n \times n}$ is unitary and S is diagonal with nonnegative and ordered entries. That is:

$$U : \ U^*U = \bar{U}^T U = I \ , \quad S = \mathrm{diag}(\sigma_1, \ldots, \sigma_n), \ \ \sigma_1 \geq \cdots \geq \sigma_n \geq 0 \ .$$

The values $\sigma_1, \ldots, \sigma_n$ are the singular values of A and S is indeed the standard matrix Σ in the SVD of A (see below).

The Takagi factorization has been used in the study of inhomogeneous plane waves in [10], it has shown to be of relevance in the quantum mechanical formulation of decay phenomena in [15], and it has also recently been used in the Physics literature in connection to the Bloch-Messiah reduction, to which is effectively equivalent; see [2] and [12], and we note that the latter work is in particular interested in studying the structural changes brought upon by degeneracies (i.e., multiple singular values), which is precisely the topic we address in the present work.

We next state a result about the existence of a Takagi factorization of a symmetric matrix, further clarifying the degree of uniqueness of the factorization. For the existence we refer to [11], [2] or [1] (where it is called *symmetric SVD*), whereas, for the degree of uniqueness, we remark that it is the same as that of the unitary factors in the SVD.

Lemma 1.1 (Takagi Factorization).

Existence. *Let $A \in \mathbb{C}^{n \times n}$ be symmetric: $A = A^T$. Then, A admits a Takagi factorization $A = USU^T$, where U is unitary and S is the diagonal matrix of singular values of A, which we will take to be ordered: $S = \mathrm{diag}(\sigma_1, \ldots, \sigma_n)$, $\sigma_1 \geq \cdots \geq \sigma_n \geq 0$.*

Uniqueness. *Next, let $A = QSV^*$ be an SVD of A. Assume that there are p distinct singular values σ_j, of multiplicity n_j, $j = 1, \ldots, p$, so that $S = \mathrm{diag}(\sigma_1 I_{n_1}, \ldots, \sigma_p I_{n_p})$, $n_1 + \cdots + n_p = n$. Then, all possible Takagi factorizations are obtained by choosing $U = QK$, where K is a block-diagonal unitary matrix, $K = \begin{bmatrix} K_{11} & & \\ & \ddots & \\ & & K_{pp} \end{bmatrix}$, and each $K_{jj} \in \mathbb{C}^{n_j \times n_j}$ is unitary ($K_{jj}^* K_{jj} = I_{n_j}$, $j = 1 \ldots, p$). Moreover, relative to the nonzero singular values, K_{jj} must satisfy $K_{jj}^2 = \bar{H}_{jj}$, where $H = V^T Q$, whereas if $\sigma_p = 0$, then K_{pp} can be any unitary matrix in $\mathbb{C}^{n_p \times n_p}$.*

It must be noted that in Lemma 1.1 any unitary square root K_{jj} of $\bar{H}_{jj}$ can be selected to obtain a Takagi factorization.

Finally, below we give a simple algorithm, Algorithm 1.1, to obtain a Takagi factorization when A is nonsingular and with distinct singular values. The construction below was proposed in [11, Exercise 15, p.423] and further used in [3], to obtain the Takagi factorization of A, and is based on the SVD of A. An alternative numerical method is given in [18].

Algorithm 1.1: Takagi factorization via the SVD

Input: $A \in \mathbb{C}^{n \times n}$ nonsingular, symmetric: $A = A^T$, and with distinct singular values.

Output: $U \in \mathbb{C}^{n \times n}$ unitary, and $S = \mathrm{diag}(\sigma_1, \ldots, \sigma_n)$, such that $\sigma_1 > \sigma_2 > \cdots > \sigma_n > 0$ and $A = USU^T$.

1. Let $A = U\Sigma V^*$ be the SVD of A with $U, V \in \mathbb{C}^{n \times n}$ unitary, and ordered singular values in Σ. Let $S = \Sigma$ and observe that $U^* A \bar{U}$ is diagonal.

2. Let $\Phi = \mathrm{diag}(\phi_1, \ldots, \phi_n)$, where $\phi_k \in \mathbb{R}$, and solve the system $\Sigma e^{2i\Phi} = U^* A \bar{U}$ to obtain $e^{2i\phi_k} = \frac{(U^* A \bar{U})_{kk}}{\sigma_k}$, $k = 1, \ldots, n$. Take a square root of $e^{2i\Phi}$ and obtain $e^{i\Phi}$. (Any complex square root is a legitimate choice).

3. Correct the unitary factor U: $U \leftarrow U e^{i\Phi}$.

Remark 1.2. Note that, in case A is invertible and has distinct singular values, the factors S and U in a Takagi factorization of A are unique up to the signs of the columns of U.

In this work we are interested in studying the Takagi factorization of a complex and symmetric matrix valued function **smoothly depending on parameters**. We will be

concerned with two issues: (i) smoothness of the factors, and (ii) degenerate (i.e., multiple or zero) singular values. In the latter case, we will also device (and test) numerical methods to find the parameter values where degeneracies occur. A plan of the paper is as follows. In Section 2 we will discuss the general concern of smoothness with respect to parameters, and the crucially important concern of the co-dimension of having a pair of degenerate singular values, showing that the co-dimension is 2 both for equal singular values and a zero singular value. In Section 3 we will look at the 1-parameter case, derive differential equations for the factors, and further use these in the context of a predictor-corrector algorithm to compute a smooth path of Takagi factorizations. Finally, in Section 4 we report on numerical experiments aimed at computing parameter values where matrices smoothly depending on 2 parameters have degenerate singular values.

2. Smoothness results, degenerate singular values, co-dimension.

We first give a general result on the co-dimension of having multiple singular values, or a 0 singular value. Before proceeding, we point out that, throughout the work, dimension of vectors spaces and manifolds will always be understood to be the real dimension.

Theorem 2.1. *Consider $A \in \mathbb{C}^{n \times n}$, symmetric. Then, having two equal nonzero singular values is a co-dimension 2 phenomenon. Furthermore, having one singular value equal to 0 is also a co-dimension 2 phenomenon.*

Proof. Note that the dimension of the space of complex symmetric matrices is $2(n(n-1)/2 + n) = n^2 + n$. Now, let $A = USU^T$ be a Takagi factorization of A.

The set W of complex symmetric matrices with a double singular value is the image of the map $(U, S) \to USU^T$, where U is unitary and $S = \mathrm{diag}(\sigma_1, \ldots, \sigma_n)$ has two equal nonzero diagonal entries. Without loss of generality, we can assume $\sigma_1 = \sigma_2$. The dimension of the manifold of unitary matrices is n^2. But, if we take $\tilde{U} = UQ$, with $Q = \begin{bmatrix} c & s \\ -s & c \\ & & I_{n-2} \end{bmatrix} \in \mathbb{R}^{n \times n}$, where $c^2 + s^2 = 1$, then $\tilde{U}S\tilde{U}^T = USU^T$ and $\tilde{U}$ is still unitary. Hence the maximum dimension of the strata of W is $n^2 - 1 + n - 1 = n^2 + n - 2$. Thus, W has co-dimension two.

Next, consider the set W of complex symmetric matrices with a 0 singular value. This is the image of the map $(U, S) \to USU^T$, where U is unitary and the diagonal S has $\sigma_n = 0$. If we now take $\tilde{U} = UQ$, $Q = \begin{bmatrix} I_{n-1} & \\ & \eta \end{bmatrix} \in \mathbb{C}^{n \times n}$, where $|\eta| = 1$, then $\tilde{U}S\tilde{U}^T = USU^T$ and $\tilde{U}$ is unitary. Hence the maximum dimension of the strata of W is $n^2 + n - 1 - 1 = n^2 + n - 2$. Thus, also in this case W has co-dimension two. $\square$

Remarks 2.2.

(i) The result of Theorem 2.1 is surprising, because we recall (see [6, p. 818]) that, for a general $A \in \mathbb{C}^{n \times n}$, having a pair of equal singular values is a co-dimension 3 phenomenon! We note that when $A \in \mathbb{R}^{n \times n}$, having two equal singular values is a co-dimension 2 phenomenon, and hence the impact of symmetry in this complex case is to lower the co-dimension of having two equal singular values to be like in the real case.

(ii) This lowering of co-dimension phenomenon does not occur insofar as loss of rank
     (0 singular value) is concerned. Indeed, also for a general $A \in \mathbb{C}^{n \times n}$, having a
     0 singular value is a co-dimension 2 phenomenon (because $\det(A)$ is a complex
     number and, in general, $\det(A) = 0$ amounts to two independent conditions).
     However, for $A \in \mathbb{R}^{n \times n}$ having a 0 singular value is a co-dimension 1 phenomenon
     (because $\det(A)$ is real). So, the impact of symmetry in this complex case is not
     to bring the co-dimension of having a 0 singular value to be equal to that of the
     real case.

(iii) It must be appreciated that, for a complex symmetric matrix, having a pair of
      singular values not just equal **but** equal to a specific value is a higher co-dimension
      occurrence. For example, having a pair of 0 singular values is a phenomenon of
      co-dimension 6! ($A = A^T = \begin{bmatrix} a & b \\ b & c \end{bmatrix} \in \mathbb{C}^{2 \times 2}$ has two 0 singular values if and only if
      $a = b = c = 0$, which amounts to 6 independent conditions.)

An implication of Theorem 2.1 is that, generically, 1-parameter functions will have
no double singular value, and will be full rank. For this reason, we next show that a
smooth full rank A with distinct singular values has a Takagi factorization with smooth
factors. To prove this result, we will need the following elementary result stating that a
smooth complex valued function of real variable, of modulus 1, has a smooth square root
of modulus 1.

Lemma 2.3. *Let $\eta \in \mathcal{C}^k(\mathbb{R}, \mathbb{C})$, $k \geq 1$ (or even $\eta \in \mathcal{C}^\omega$, i.e., analytic), be of modulus 1 for
all $t \in \mathbb{R}$. Then, there exists a square root function $s \in \mathcal{C}^k(\mathbb{R}, \mathbb{C})$ of modulus 1 such that
$s^2 = \eta$; s is unique up to sign.*

Proof. This is a consequence of the fact that there is a unique smooth logarithm of $\eta(t)$,
that is a unique smooth real valued function $\psi(t)$ so that $\eta(t) = e^{i\psi(t)}$, from which we will
have $s(t) = e^{i\psi(t)/2}$. $\qquad\square$

Theorem 2.4. *Let $A \in \mathcal{C}^k(\mathbb{R}, \mathbb{C}^{n \times n})$ with $k \geq 0$, $A^T = A$, and suppose that for any given
t the singular values are distinct and positive. Then, A admits a Takagi factorization,
$A(t) = U(t)S(t)U^T(t)$, $\forall t$, with U unitary and $S = \mathrm{diag}(\sigma_1, \ldots, \sigma_n)$, $\sigma_1 > \cdots > \sigma_n > 0$,
where U, S are as smooth as A.*

Proof. The result is a consequence of the construction given in Algorithm 1.1, under the
present assumptions. In fact, see [6], functions with distinct singular values have an SVD
with factors as smooth as A; that is, in the decomposition $A(t) = U(t)\Sigma(t)V^*(t)$, U, Σ, V
are as smooth as A. In particular, the diagonal function $D = \mathrm{diag}\left(\frac{(U^*A\bar{U})_{kk}}{\sigma_k}, \ k = 1, \ldots, n\right)$,
is as smooth as A and unitary. Then, using Lemma 2.3, we take a smooth square root of
the entries on the diagonal of D and obtain the stated smoothness result. $\qquad\square$

Remark 2.5. Under the assumption of Theorem 2.4, we observe that there is no freedom
left in specifying the factors of the Takagi factorization, aside from a trivial change in sign
of the columns of U. If we fix a reference Takagi factorization at some value, say at $t = 0$,
then there is only one $\mathcal{C}^k$ factorization passing through these given conditions.

The most important consequence of Theorem 2.1 is that we need to consider functions of 2 real parameters to expect having a pair of equal singular values or a zero singular value. This is the same situation as what we have for coalescing singular values in the real (not complex) case; e.g., see [9]. Furthermore, these occurrences are expected to take place at isolated parameter values, and to persist under generic perturbations. For these reasons, below we will focus on matrices depending (smoothly) on two parameters and we will address the concerns of locating parameter values where there are double singular values or where a singular value vanishes. We will call *conical intersections* the locations where two singular values become equal.

We next see that –similarly to the real symmetric eigenproblem– the columns of U associated to a pair coalescing eigenvalues will undergo a change in sign (they flip over) when we cover a loop (i.e., a closed curve) in parameter space, enclosing the associated conical intersection. Similarly, we will see that the column of U associated to a 0 singular value inside the loop will undergo a change in sign as we cover the loop. As previously remarked, we should not be concerned with the possibility of encountering a conical intersection, or a 0 singular value, as we cover the 1-d loop, since coalescings and losses of rank are co-dimension 2 phenomena, not 1.

To obtain the result on coalescing singular values, and losses of rank, we adopt the following rewriting (e.g., used in [5, Theorem 2.7]). We write $A \in \mathbb{C}^{n \times n}$, $A = A^T$, as $A = B + iC$, $B, C \in \mathbb{R}^{n \times n}$ symmetric. Then, we associate to A the following (special) symmetric matrix $M \in \mathbb{R}^{2n \times 2n}$:

$$(1) \qquad M = \begin{bmatrix} B & C \\ C & -B \end{bmatrix} , \quad B = B^T , \quad C = C^T .$$

Now we make the following observations.

(i) The eigenvalues of M are given by $\mathrm{diag}(S)$ and $\mathrm{diag}(-S)$ (i.e., the singular values of A and their opposite values). We will label the eigenvalues of M as $\lambda_1 \geq \ldots \lambda_n \geq \lambda_{n+1} \geq \cdots \geq \lambda_{2n}$, where $\lambda_j = \sigma_j$, and $\lambda_{n+j} = -\sigma_{n-j+1}$, $j = 1, \ldots, n$.

(ii) If U is a unitary Takagi factor of A, writing $U = V + iZ$, then $W = \begin{bmatrix} V & Z \\ Z & -V \end{bmatrix}$ gives an orthogonal eigendecomposition of M: $W^T M W = \begin{bmatrix} S & 0 \\ 0 & -S \end{bmatrix}$. Vice versa, if $M \begin{bmatrix} X \\ Y \end{bmatrix} = \begin{bmatrix} X \\ Y \end{bmatrix} S$, with $\begin{bmatrix} X \\ Y \end{bmatrix}$ orthonormal, then also $M \begin{bmatrix} Y \\ -X \end{bmatrix} = \begin{bmatrix} Y \\ -X \end{bmatrix} (-S)$, $W = \begin{bmatrix} X & Y \\ Y & -X \end{bmatrix}$ is an orthogonal eigendecomposition of M, and $U = X + iY$ is unitary and gives a Takagi factorization of A.

In light of the correspondence just outlined between the Takagi factors and the symmetric eigenproblem, see (1), we can now exploit known results about conical intersections of eigenvalues of symmetric functions of two parameters to obtain the corresponding results for the coalescing singular values of a Takagi factorization. We give the main result in the

next theorem, whose proof amounts to putting together known results for the symmetric eigenproblem, relative to *generic* coalescing points; we refer to [9] for the meaning of generic in this context[1], and we note that to say that the smallest eigenvalue vanishes at a generic point means that the ordered n-th and $(n+1)$-st eigenvalues of M have a generic coalescing there.

Theorem 2.6. *Let $A \in \mathcal{C}^k(\Omega, \mathbb{C}^{n \times n})$ with $k \geq 0$, $A^T = A$, and Ω a closed and bounded subset of $\mathbb{R}^2$. Let $\sigma_1 \geq \cdots \geq \sigma_n \geq 0$ be the continuous singular values of A in Ω. Let Γ be a simple closed curve in Ω, parametrized as a smooth function $\gamma(t)$, $t \in [0,1]$, and assume that the singular values of A are nonzero and distinct along Γ. Let $A(t) = A(\gamma(t))$, $t \in [0,1]$, be the restriction of A to Γ. Let $A(0) = U_0 S_0 U_0^T$ be a given Takagi factorization of $A(0)$, and let $U(t)$, $S(t)$, be the unique smooth Takagi factors of $A(t)$, for all $t \in [0,1]$, satisfying $U(0) = U_0$, $S(0) = S_0$. Partition $U(t) = \begin{bmatrix} u_1(t) & \ldots & u_n(t) \end{bmatrix}$.*

Finally, assume that there is a unique, generic, coalescing point $x \in \Omega$, where $\sigma_j = \sigma_{j+1}$, for some $j = 1, \ldots, n-1$, and that there is no other point in Ω where a pair of singular values coalesce or a singular value is zero. Then,

$$(2) \quad u_k(1) = u_k(0)\,, \quad \text{for} \quad k \neq j, j+1\,, \quad \text{and} \quad \begin{bmatrix} u_j(1) & u_{j+1}(1) \end{bmatrix} = -\begin{bmatrix} u_j(0) & u_{j+1}(0) \end{bmatrix}\,.$$

Similarly, if σ_n vanishes at a unique, generic, point inside Ω, and it is $\sigma_n \neq \sigma_{n-1}$ in Ω, then $u_n(1) = -u_n(0)$.

Proof. Under the given hypotheses, the function M in Ω has the continuous and ordered eigenvalues $\lambda_1 = \sigma_1 \geq \cdots \geq \lambda_n = \sigma_n \geq \lambda_{n+1} = -\sigma_n \geq \cdots \geq \lambda_{2n} = -\sigma_1$, and along Γ these are distinct and $\lambda_1 > \cdots > \lambda_n > 0 > \lambda_{n+1} > \cdots > \lambda_{2n}$.

Now, in the case of two equal singular values at a generic point $x \in \Omega$, we will have both $\lambda_j(x) = \lambda_{j+1}(x)$ and $\lambda_{2n-j+1}(x) = \lambda_{2n-j}(x)$ (since the latter are the negative of the singular values). Then, appealing to Theorem 3.3 in [9] for two pairs of coalescing eigenvalues of symmetric functions, given the form (1), and noticing that a coalescing must occur within the first n ordered eigenvalues of M, we obtain the desired result: $\begin{bmatrix} u_j(1) & u_{j+1}(1) \end{bmatrix} = -\begin{bmatrix} u_j(0) & u_{j+1}(0) \end{bmatrix}$.

As far as the vanishing singular value, we again reason with the enlarged system (1), and now notice that a 0 singular value reflects in the coalescing pair λ_n and λ_{n+1} as eigenvalues of M. In this case, we can appeal to Theorem 2.8 of [9] to conclude that $u_n(1) = -u_n(0)$. $\qquad\square$

Remark 2.7. Again by appealing to the enlarged system (1), the case of multiple (generic) points of degeneracy of the singular values in Ω can be analyzed similarly to the way that multiple points of coalescence for eigenvalues were dealt with in [9], to which we refer for details. In essence, one can show that each generic degeneracy causes the eigenvector(s) involved in the degeneracy to change sign (see Eq. (2)). For instance, suppose that $\sigma_1 = \sigma_2$ and $\sigma_2 = \sigma_3$ at two distinct generic coalescing points in Ω, and that there are no other points of degeneracy for the singular values in Ω. Then, the eigenvectors $u_1(t), u_2(t), u_3(t)$

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[1]In essence, it means that the surfaces of eigenvalues of M come together as a double cone at points where the eigenvalues are equal.

smoothly continued around a 1-periodic loop that contains the two coalescing points will satisfy:

$$\begin{bmatrix} u_1(1) & u_2(1) & u_3(1) \end{bmatrix} = \begin{bmatrix} -u_1(0) & u_2(0) & -u_3(0) \end{bmatrix},$$

because both pairs u_1, u_2 and u_2, u_3 will change sign. Similarly, if $\sigma_{n-1} = \sigma_n$ and $\sigma_n = 0$ at two distinct points and $\sigma_1 > \cdots > \sigma_n > 0$ elsewhere, then:

$$\begin{bmatrix} u_{n-1}(1) & u_n(1) \end{bmatrix} = \begin{bmatrix} -u_{n-1}(0) & u_n(0) \end{bmatrix}.$$

3. ONE PARAMETER CASE.

As we saw, under the conditions of Theorem 2.4, a 1-parameter function A admits a smooth Takagi factorization. Next, we are going to derive differential equations describing the evolution of the factors U and S, and then we will give an algorithm to compute a smooth Takagi factorization for 1-parameter functions, under the assumption of distinct and nonzero singular values.

3.1. **Differential equations for the factors.** From here on, we will use the notation $\dot{y}$ to indicate the derivative of a function $y = y(t)$ with respect to t. We have the following result.

Theorem 3.1. *Let $A \in \mathcal{C}^k([0, \infty), \mathbb{C}^{n \times n})$ with $k \geq 0$, and let $A^T = A$. Suppose that for any given $t \geq 0$ the singular values of $A(t)$ are distinct and positive. Let $A(0) = U_0 S_0 U_0^T$ be a Takagi factorization at $t = 0$. Then, the smooth factors U and S for which $A(t) = U(t)S(t)U^T(t)$, for all $t \geq 0$, with U unitary, $S = \mathrm{diag}(\sigma_1, \ldots, \sigma_n)$, $\sigma_1 > \cdots > \sigma_n > 0$, $U(0) = U_0$ and $S(0) = S_0$, satisfy the differential equations*

$$\dot{S} = \mathrm{Re}(\mathrm{diag}(U^* \dot{A} \bar{U}))$$

(3)

$$\dot{U} = UH \ ,$$

where $H = U^* \dot{U}$ is the skew-Hermitian function such that

(4)
$$H_{kk} = i \frac{\mathrm{Im}(U^* \dot{A} \bar{U})_{kk}}{2\sigma_k} \ , \qquad k = 1, \ldots, n \ ,$$

$$H_{kj} = \frac{\mathrm{Re}(U^* \dot{A} \bar{U})_{kj}}{\sigma_j - \sigma_k} + i \frac{\mathrm{Im}(U^* \dot{A} \bar{U})_{kj}}{\sigma_j + \sigma_k} \ , \qquad k = 1, \ldots, n \ , \ j = 1, \ldots, k-1 \ .$$

Proof. We differentiate the relation $A(t) = U(t)S(t)U^T(t)$ to obtain

$$\dot{A} = \dot{U}SU^T + U\dot{S}U^T + US\dot{U}^T$$

$$U^* \dot{A} \bar{U} = U^* \dot{U} S U^T \bar{U} + U^* U \dot{S} U^T \bar{U} + U^* U S \dot{U}^T \bar{U}.$$

Now, using $U^* U = I$ (hence $U^T \bar{U} = I$), and letting $H = U^* \dot{U}$ which is skew-Hermitian and hence $\dot{U}^T \bar{U} = -\bar{H}$, we have

(5)
$$\dot{S} = U^* \dot{A} \bar{U} - HS + S\bar{H} \ , \qquad \dot{U} = UH \ .$$

Now we use the fact that S is diagonal, $S = \mathrm{diag}(\sigma_k, \ k = 1, \ldots, n)$, to obtain for the singular values

$$\dot{\sigma}_k = (U^* \dot{A} \bar{U})_{kk} - H_{kk} \sigma_k + \sigma_k \bar{H}_{kk} \quad \text{or}$$

$$\dot{\sigma}_k = (U^* \dot{A} \bar{U})_{kk} - 2 H_{kk} \sigma_k \ .$$

Now, we must have $H_{kk} = i\phi_k$, where $\phi_k \in \mathbb{R}$, and $\sigma_k \in \mathbb{R}$. So, we let $(U^* \dot{A} \bar{U})_{kk} = \alpha_{kk} + i\beta_{kk}$ and thus obtain $\dot{\sigma}_k = \alpha_{kk} + i(\beta_{kk} - 2\phi_k \sigma_k)$ and so

$$(6) \qquad\qquad \dot{\sigma}_k = \alpha_{kk} \ , \quad \phi_k = \frac{\beta_{kk}}{2\sigma_k} \ , \quad k = 1, \ldots, n \ .$$

At the same time we must have $(\dot{S})_{kj} = 0$, $k \neq j$, and we will use this to obtain the remaining relations for the entries of H. Namely, we have

$$(U^* \dot{A} \bar{U})_{kj} - H_{kj} \sigma_j + \sigma_k \bar{H}_{kj} = 0$$

and letting $H_{kj} = \alpha_{kj} + i\beta_{kj}$ we have

$$(U^* \dot{A} \bar{U})_{kj} = \alpha_{kj}(\sigma_j - \sigma_k) + i\beta_{kj}(\sigma_j + \sigma_k)$$

and therefore

$$(7) \quad \alpha_{kj} = \frac{\mathrm{Re}(U^* \dot{A} \bar{U})_{kj}}{\sigma_j - \sigma_k} \ , \quad \beta_{kj} = \frac{\mathrm{Im}(U^* \dot{A} \bar{U})_{kj}}{\sigma_j + \sigma_k} \ , \qquad k = 1, \ldots, n \ , \ \ j = 1, \ldots, k-1 \ .$$

Using (6) and (7) in (5), we obtain the differential equations governing the evolution of the factors S and U in the Takagi factorization of A. $\qquad\qquad\square$

Remark 3.2. The assumption of nonzero singular values has been used in (6) to obtain uniquely the phases ϕ_k's. The assumption of distinct singular values has been used in (7) to obtain the values H_{kj}.

3.2. **A predictor corrector algorithm to compute the factorization along loops in parameter space.** Following the lines of our previous work on eigenvalue problems, see [8], we developed a predictor-corrector procedure to compute the smooth Takagi factorization of one parameter symmetric functions.

Given the factorization $A(t) = U(t)S(t)U^T(t)$ at some t, we briefly describe how we compute the smooth factors U and S at a new point $t_{new} = t + h$. The diagonal factor $S(t_{new})$ and a unitary matrix U_{new} such that $A(t_{new}) = U_{new} S(t_{new}) U_{new}^T$ are obtained by Algorithm 1.1, using standard software like the MATLAB `svd` command. Recalling that U_{new} is unique up to the signs of its columns, correct signs for $U(t_{new})$ can be predicted using the differential equations. Indeed, taking an Euler step in (3)-(4), we first have

$$U(t + h) \simeq U(t)(I + hH(t)).$$

Since $H(t)$ depends on the matrix $U^*(t)\dot{A}(t)\bar{U}(t)$, we replace the derivative $\dot{A}(t)$ with $(A(t + h) - A(t))/h$,

$$U^*(t)\dot{A}(t)\bar{U}(t) \simeq \frac{U^*(t)A(t + h)\bar{U}(t) - S(t)}{h}.$$

Upon realizing that the term $S(t)/h$ (which is real and diagonal) is irrelevant in obtaining the expressions for H_{kk} and H_{kj}, we set $A_U = U^*(t)A(t+h)\bar{U}(t)$ and finally have

$$U^{pred} = U(t)(I + \mathcal{H}), \quad \text{with } \mathcal{H} \text{ skew-Hermitian and such that}$$

(8)
$$\mathcal{H}_{kk} = i\frac{\text{Im}(A_U)_{kk}}{2\sigma_k} , \quad k = 1, \ldots, n ,$$

$$\mathcal{H}_{kj} = \frac{\text{Re}(A_U)_{kj}}{\sigma_j - \sigma_k} + i\frac{\text{Im}(A_U)_{kj}}{\sigma_j + \sigma_k} , \quad k = 1, \ldots, n , \; j = 1, \ldots, k-1 .$$

Then, we compute the sign matrix $Z = \text{sign}(\text{Re}(\text{diag}(U^*_{new} U^{pred})))$ to correct the signs of the singular vectors, and set $U(t_{new}) = U_{new} Z$. Clearly, the correction is reliable as long as the stepsize h is sufficiently small with respect to factors variation, which we monitor by computing the following parameters:

(9)
$$\rho_U = \frac{\left\|U(t_{new}) - U^{pred}\right\|_F}{\sqrt{n}} \quad \text{and} \quad \rho_\sigma = \max_j \frac{\left|\sigma_j(t_{new}) - \sigma_j^{pred}\right|}{|\sigma_j(t_{new})| + 1} ;$$

predicted singular values σ_j^{pred}, $j = 1, \ldots, n$, are obtained proceeding as before for U^{pred}:

(10)
$$S(t+h) \simeq S(t) + h \, \text{Re}(\text{diag}(U^*(t)\dot{A}(t)\bar{U}(t))) \simeq \text{Re}(\text{diag}(A_U)) \equiv S^{pred}.$$

We show in Algorithm 3.1 how ρ_U and ρ_σ are used to update the stepsize h (see Step 4), and to accept a step or declare *failure* (see Step 5).

Finally, before attempting a new step after an accepted one, we use the following simple secant approximation of the singular values at $t_{new} + h$:

$$\sigma_j^{sec} = \sigma_j(t_{new}) + h \, \dot{\sigma}_j^{sec} = \sigma_j(t_{new}) + h \, \frac{\sigma_j(t_{new}) - \sigma_j(t)}{t_{new} - t} \simeq \sigma_j(t_{new} + h), \quad j = 1, \ldots, n,$$

in order to reduce the occurrence of failures. Recall that we expect to have $\sigma_1 > \sigma_2 > \ldots > \sigma_n > 0$: then the new step $t_{new} + h$ is likely to fail if either $\sigma_n^{sec} < 0$ or $\sigma_j^{sec} < \sigma_{j+1}^{sec}$ for some j. In these cases h is reduced - at least halved - as shown at Steps 7 and 8 of Algorithm 3.1.

Following a smooth path can typically force the algorithm to take small steps, possibly very small steps, when it passes near a point where either σ_n vanishes or two singular values coalesce, depending on the distance from such degeneracies. This behaviour is easily justified looking again at the differential equations (3)-(4). Indeed, since H_{nn} and the real part of the matrix H are inversely proportional, respectively, to σ_n and to the difference between two singular values, when one of these quantities is small some rapid variation in the unitary factor U has to be expected. A lower bound h_{min} for the stepsize is then recommended, below which the continuation procedure has to be halted. In our experiments we set $h_{min} = 100 \, \texttt{eps}$, where $\texttt{eps} = 2^{-52}$ is the default machine precision in MATLAB.

Algorithm 3.1: Predictor-Corrector step

Input: t, the Takagy factorization $A(t) = U(t)S(t)U^T(t)$, stepsize h, tolerance `tolstep`.

Output: t_{new}, the smooth factors $U(t_{new})$ and $S(t_{new})$, an updated stepsize h.

1. Set $t_{new} = t + h$, and compute U^{pred} and S^{pred} by (8) and (10);
2. Compute a Takagi factorization $A(t_{new}) = U_{new} S(t_{new}) U_{new}^T$ by Algorithm 1.1;
3. Set $U(t_{new}) = U_{new} Z$, with $Z = \text{sign}(\text{Re}(\text{diag}(U_{new}^* U^{pred}))$;
4. Compute ρ_σ and ρ_U from (9), set $\rho = \max\{\rho_\sigma, \rho_U\}/$`tolstep`, and update $h = h/\rho$;
5. If $\rho \leq 1.5$, accept the step;
   otherwise declare *failure*, go to step 1, and retry with the new (smaller) h;
6. Compute $\dot{\sigma}_j^{sec} = \dfrac{\sigma_j(t_{new}) - \sigma_j(t)}{t_{new} - t}$ and $\sigma_j^{sec} = \sigma_j(t_{new}) + h\dot{\sigma}_j^{sec}$, for $j = 1, \ldots, n$;
7. If $\sigma_j^{sec} < \sigma_{j+1}^{sec}$ for some $j = 1, \ldots, n-1$, set $h = \min\{h/2, 0.9\, h_{sec}\}$, where

$$h_{sec} = \min\left\{ \frac{\sigma_j(t_{new}) - \sigma_{j+1}(t_{new})}{\dot{\sigma}_{j+1}^{sec} - \dot{\sigma}_j^{sec}}, \text{ for } \sigma_j^{sec} < \sigma_{j+1}^{sec}, \ j = 1, \ldots, n-1 \right\};$$

8. If $\sigma_n(t_{new}) + h\dot{\sigma}_n^{sec} < 0$, set $h = \min\{h/2, 0.9\, \sigma_n(t_{new})/|\dot{\sigma}_n^{sec}|\}$.

---

4. Complex symmetric random matrices and numerical tests.

We should appreciate that the sole knowledge that the co-dimension of having degenerate singular values is 2 does not give any insight into how many coalescing points we should expect to have in a spatial region of parameter space. Yet, the latter is exactly the kind of knowledge that one wants: how many isolated coalescings should we expect? For this reason, the goal of this section is to provide some insight into the so-called *density of degeneracies* for the Takagi factorization, relative to an appropriate ensemble of random matrices depending on two parameters.

In our experiments, we built several realizations of 2-parameter matrix valued functions of increasing size, and performed a statistical study on the number of coalescings and losses of rank found in a certain domain. Our matrix valued functions are defined as trigonometric combinations of four matrices $A_1, \ldots, A_4$:

(11) $A(x, y) = A_1 \cos(x) + A_2 \sin(x) + A_3 \cos(y) + A_4 \sin(y), \ (x, y) \in \mathbb{R}^2,$

where each matrix A_k is generated as follows:

(1) take a random matrix $B \in \mathbb{C}^{n \times n}$ with entries $B_{ij} = x_{ij} + i\, y_{ij}$, where x_{ij} and y_{ij} are i.i.d. selected from $N_{\mathbb{R}}(0, \frac{1}{4})$,

(2) form $A_k = B + B^T$.

Matrix functions like (11) had been considered in [17] in a study of degeneracies for real symmetric random matrices. Note that a function $A(x, y)$ like in (11) is defined (and analytic) everywhere in $\mathbb{R}^2$. Moreover, being each matrix A_k symmetric with off-diagonal

entries in $N_{\mathbb{C}}(0,1)$ and diagonal entries in $N_{\mathbb{C}}(0,2)$, the same is true for $A(x,y)$ for all values of x and y, except that the variances are two times those of the corresponding entries of the matrices A_k's.

Hereafter, we will denote by $\mathcal{G}$ the ensemble of random symmetric matrices of interest, defined as follows:

$$\mathcal{G} = \left\{ A \in \mathbb{C}^{n \times n} : \ A = A^T = (A_{ij})_{i,j=1}^n \text{ such that } \left\{ \begin{array}{ll} a_{ij} \in N_{\mathbb{C}}(0,2) & \text{if } i = j \\ a_{ij} \in N_{\mathbb{C}}(0,1) & \text{otherwise} \end{array} \right\} \right. .$$

Theorem 4.1. *Let $U \in \mathbb{C}^{n \times n}$ be unitary. Then, if $A \in \mathcal{G}$, also $U^T A U \in \mathcal{G}$.*

Proof. Let $A \in \mathcal{G}$. It is straightforward to see that all entries of $U^T A U$ are normally distributed with mean zero. Let us compute their variances.

Diagonal entries: Let $1 \leq i \leq n$. Then we have:

$$\left(U^T A U\right)_{ii} = \sum_{h,k=1}^n A_{hk} U_{hi} U_{ki} = \sum_{h=1}^n A_{hh} U_{hi}^2 + 2 \sum_{\substack{h,k=1 \\ h<k}}^n A_{hk} U_{hi} U_{ki} .$$

Given that all entries along and above the diagonal of A are independent, we have:

$$\text{var}\left(\left(U^T A U\right)_{ii}\right) = \sum_{h=1}^n \text{var}\left(A_{hh}\right) |U_{hi}|^4 + 4 \sum_{\substack{h,k=1 \\ h<k}}^n \text{var}\left(A_{hk}\right) |U_{hi}|^2 |U_{ki}|^2$$

$$= 2 \left(\sum_{h=1}^n |U_{hi}|^4 + 2 \sum_{\substack{h,k=1 \\ h<k}}^n |U_{hi}|^2 |U_{ki}|^2 \right) = 2 \left\| U_{:,i} \left(U_{:,i}\right)^* \right\|_F^2 = 2 ,$$

where $U_{:,i}$ denotes the i-th column of U.

Off-diagonal entries: Let $i, j = 1, \ldots, n$, $i \neq j$. We have:

$$\left(U^T A U\right)_{ij} = \sum_{h,k=1}^n A_{hk} U_{hi} U_{kj} = \sum_{h=1}^n A_{hh} U_{hi} U_{hj} + \sum_{\substack{h,k=1 \\ h<k}}^n A_{hk} \left(U_{hi} U_{kj} + U_{ki} U_{hj}\right) .$$

Just as before, we can compute the variance of $\left(U^T A U\right)_{ij}$:

$$\text{var}\left(\left(U^T A U\right)_{ij}\right) = \sum_{h=1}^n \text{var}\left(A_{hh}\right) |U_{hi}|^2 |U_{hj}|^2 + \sum_{\substack{h,k=1 \\ h<k}}^n \text{var}\left(A_{hk}\right) |U_{hi} U_{kj} + U_{ki} U_{hj}|^2$$

$$= 2 \sum_{h=1}^n |U_{hi}|^2 |U_{hj}|^2 + \frac{1}{2} \sum_{\substack{h,k=1 \\ h \neq k}}^n |U_{hi} U_{kj} + U_{ki} U_{hj}|^2$$

$$= \frac{1}{2} \left\| U_{:,i} \left(U_{:,i}\right)^T + U_{:,j} \left(U_{:,j}\right)^T \right\|_F^2 = 1 ,$$

□

Remark 4.2. In a sense, the ensemble $\mathcal{G}$ is a complex symmetric analog of two classes of random matrices that have been extensively studied: the Gaussian orthogonal and unitary ensembles (GOE/GUE), see [14]. It is a well known fact that matrices in the GOE and GUE ensembles are invariant under the similarities $A \mapsto U^T A U$ with U orthogonal and $A \mapsto U^* A U$ with U unitary, respectively. Computations similar to those performed in the proof of Theorem 4.1 yield the following identities for given $A \in \mathcal{G}$ and unitary $U \in \mathbb{C}^{n \times n}$:

$$\mathrm{var}\left((U^* A U)_{ii}\right) = 2\left(1 - \|\mathrm{Im}\left(U_{:,i}\left(U_{:,i}\right)^*\right)\|_F^2\right), \quad \text{for all } i = 1, \ldots, n.$$

$$\mathrm{var}\left((U^* A U)_{ij}\right) = 1, \text{ for all } i, j = 1, \ldots, n, \text{ with } i \neq j.$$

This shows that $\mathcal{G}$ is not invariant under the unitary similarity $A \mapsto U^* A U$ unless U is real, in which case we have $U^* = U^T$ and fall back into the case of Theorem 4.1.

We now report on the results of our experiments. We carried out two different sets of experiments, aimed at counting the number of points within a given region Ω where, respectively, a pair of singular values coalesces and a loss of rank occurs. To study the coalescence of singular values, we built 10 realizations of random matrix functions defined as in (11) for each of the following dimensions: $50, 60, \ldots, 120$. For the losses of rank, we built 20 realizations for each of the dimensions $50, 100, \ldots, 500$. Because of periodicity of $A(x, y)$, we took the domain $\Omega = [0, 2\pi] \times [0, \pi]$. We divided Ω into a uniform grid made of 1024×512 square boxes and, for each box, we established the presence of a coalescing point of singular values by numerically verifying the change of sign expressed through equation (2) in Theorem 2.6. In practice, the verification is based upon the computation of a smooth Takagi factorization around the sides of each box through the algorithm described in Section 3.2, where we have set $\texttt{tolstep} = 10^{-2}$. For the losses of rank, we actually chose a coarser grid of 128×64 boxes, since in this case we observed a much smaller number of events and had to increase the dimension of the problems in order to obtain statistically relevant data. To establish the occurrence of a loss of rank, we relied on the same tools described above but counted only the coalescing points for the pair of eigenvalues $(\lambda_n, \lambda_{n+1})$ of the $2n \times 2n$ matrix function $M(x, y)$ defined in (1). In practice, however, we did not work with the double–size matrix M, but made use of the fact that coalescence for this pair of eigenvalues of M is betrayed by an odd number of columns of U changing sign upon continuation around the boundary of a box, see Remark 2.7. All computations have been performed on PACE, the HPC infrastructure at the Georgia Institute of Technology, and required a total of about 9K CPU-hours.

The results of the experiments are illustrated in Figure 1. They suggest that the number of coalescing points of singular values grows **quadratically** in the size of the problem, and that the number of points where there is a loss of rank grows **linearly**.

Remark 4.3. In the physics literature (mostly quantum mechanics), for parameter dependent random matrices of a certain ensemble, the "density of degeneracies" is a probability distribution that provides the expected number of points of coalescence per unit of measure in parameter space. From the density of degeneracies, one can compute the total number
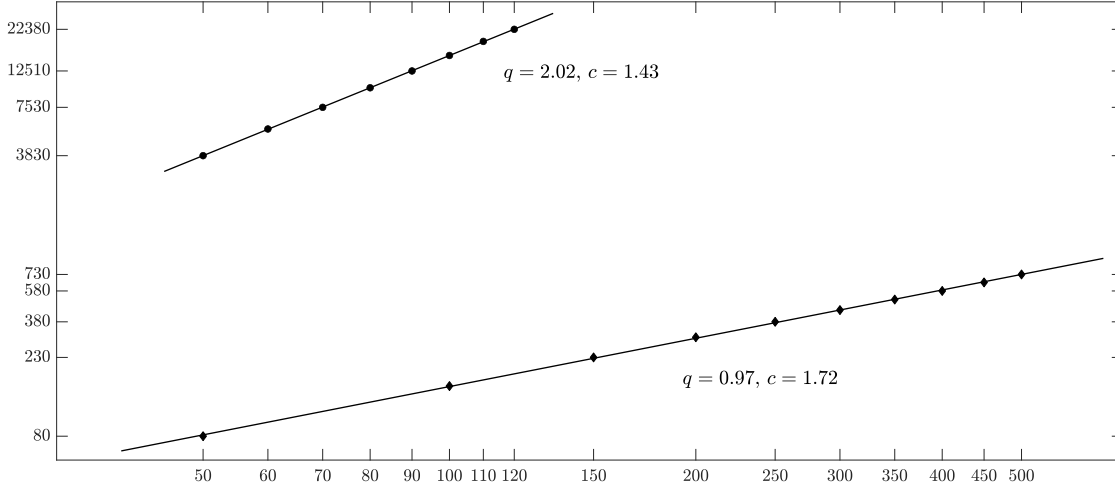
FIGURE 1. The figure shows the results of a "log–log least squares" performed on the data obtained from our experiments (circles for number of coalescences of singular values, diamonds for losses of rank). It also shows the parameters c and q obtained by best fit for the power law:

$$\text{\# of points } = c\, n^q, \text{ where } n \text{ is the matrix dimension.}$$

of points of degeneracy expected to be found within a given domain in terms of the size of the matrix functions. For the GOE and GUE ensembles, the density of degenerate eigenvalues has been computed in [17] and [16] respectively, and found to be proportional to the square (respectively, cube) of the density of eigenvalues.

We recall that, in the present work, the term "degeneracy" may refer either to coalescence of singular values or to loss of rank. Under fair working assumptions, and through an empirical argument similar to one used in [7], we make the following:

Claim 4.4. *Consider a $n \times n$ random matrix smoothly depending on two or more parameters. Assume that, for all values of the parameters, its singular values are asymptotically distributed according to the* **quarter-circle distribution**

$$(12) \qquad\qquad \rho(\sigma) = \frac{\sqrt{2}}{\pi}\sqrt{n - \sigma^2/8}, \quad \sigma \in \left[0, \sqrt{8n}\right] \ .$$

Assume that the density of coalescing singular values is given by $c\,\rho(\sigma)^p$, where $c > 0$ is a constant. Then, the expected number of points of coalescence for the singular values per unit of measure in parameter space is asymptotic to $n^{\frac{p}{2}+1}$, while the expected number of points of coalescence involving a particular pair of consecutive singular values is asymptotic to $n^{\frac{p}{2}}$. Moreover, the number of points of loss of rank is also asymptotic to $n^{\frac{p}{2}}$.

Evidence. Below we present an empirical argument in support of Claim 4.4. From (12), for the density of singular values ρ we have:

$$\int_0^{\sqrt{8n}} \rho(\sigma) \, d\sigma = n,$$

for all $n > 0$. For any $n > 2$ and any $0 \leq k \leq n$, let us consider s_k such that

$$\int_{s_k}^{\sqrt{8n}} \rho(\sigma) \, d\sigma = k.$$

Then we expect each interval $[s_k, s_{k-1}]$ to contain exactly 1 singular value of the matrix function, and also expect coalescence for a pair of consecutive singular values to occur at the boundaries of each interval. That is, we expect $\sigma_k = \sigma_{k+1} = s_k$ for $k = 1, 2, \ldots, n-1$. Therefore, given our assumption on the expression of the density of degeneracies, the expected number of coalescing points involving the pair (σ_k, σ_{k+1}) is $c\,\rho(s_k)^p = c\left(\frac{\sqrt{2}}{\pi}\right)^p \left(n - s_k^2/8\right)^{\frac{p}{2}}$, which is asymptotic to $n^{\frac{p}{2}}$, and the expected number of coalescing points involving any pair of singular values is:

$$c \sum_{k=1}^{n-1} \rho(s_k)^p = c\left(\frac{\sqrt{2}}{\pi}\right)^p \sum_{k=1}^{n-1} \left(n - s_k^2/8\right)^{\frac{p}{2}},$$

which is asymptotic to $n^{\frac{p}{2}+1}$. The reasoning on the asymptotic for the number of rank losses follows the same line, except one needs to consider the eigenvalues of the double-size problem (1). $\square$

Unfortunately, we could not find any reference for the density of singular values of random complex symmetric matrices in $\mathcal{G}$, let alone the relation between density of degenerate singular values and the density of singular values in such case. Yet, extensive numerical experiments strongly suggest that the singular values of matrices in $\mathcal{G}$ are asymptotically distributed according to the quarter-circular distribution (12). In fact, this is known to be the case for general random Gaussian matrices, and was established by Marchenko and Pastur in [13]. In the GOE/GUE cases, it is a consequence of the well known Wigner's semicircular law. Recently, it has been proved also for the so-called *checkerboard* matrices, see [4].

By virtue of Claim 4.4, the results of our experiments can be used in support of the following:

Claim 4.5. *For the random matrix functions $A(x, y)$ defined in (11), the density of coalescings for the singular values is proportional to $\rho(\sigma)^2$, where ρ is the density of singular values defined in (12).*

5. CONCLUSIONS

In this work, we considered the Takagi factorization of a matrix valued function depending on parameters. Our main interest was in being able to locate degenerate (i.e.,

double or zero) singular values in parameter space. We proved that having a generic coalescing of singular values is a co-dimension 2 phenomenon, in contrast to the case of equal singular values of a general complex matrix for which the co-dimension is 3. At the same time, losses of rank remain co-dimension 2 phenomena. We further derived a system of differential equations satisfied by a smooth factorization along 1-d paths, and proposed an algorithm of predictor-corrector type that exploits these differential equations. Finally, we implemented a method to locate the occurrence of degeneracies and made a numerical study of the density of such degeneracies, discovering that the power law governing the number of coalescing singular values is of the type $c_1 n^2$ whereas the one governing the number of losses of rank is of the type $c_2 n$, for appropriate constants c_1, c_2.

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